REMARKS/ARGUMENTS

Applicants will respond to the various items in the office action in the order they are presented.

Information Disclosure Statement

The examiner notes that the listing of references in the specification is not a proper Information Disclosure Statement. The specification reference listing was not intended to be a substitute for an Information Disclosure Statement. The references are presented as an aid to understanding the teaching set forth in the specification. Applicants are unaware of any prior art to the claims presented in this application. However, since the present application is a division of an issued parent application, for completeness of the record, Applicants will create and forward after this Response is filed an Information Disclosure Statement with the required fee setting forth all the patents which were cited in the parent.

Drawings

Applicants do not believe any changes were made to the drawings.

Specification

The examiner has objected to the specification and required appropriate correction because: "...the brief description of the drawings at pages 15-16 does not address each portion of each figure individually, as required." The amendment to the specification presented corrects the figure descriptions and brings them into conformity with the issued parent patent.

The Examiner has noted that the title of the invention is not descriptive and has required a new title that is "...clearly indicative of the invention to which the claims are directed." Applicants have amended the specification to include a revised title.

Claims

Claim Objections:

The claims have been amended to correct the informalities noted by the Examiner. Applicants have removed: 1) the periods placed after each subpart identification; and 2) the capital letters beginning each subpart. Certain other informalities in the use of a colon in place of a semi-colon were noted and corrected.

Claim Amendment to Conform Terms to Issued Patent:

The claims have been further amended to conform the claim language with respect to validated molecular descriptors to the language of the previously issued patent claims, that is; "validated molecular structural descriptors" has been amended to "molecular structural descriptors, validated as possessing a neighborhood property."

New Claims:

Applicants submit with this Response four new claims. Claims 10, 11, and 12 are similar to the initially filed claims but use the more extensive language found in the preamble to the parent patent claims to describe the virtual library. This language highlights the structural purpose of the virtual library. Claim 13 is a system claim which sets forth the implementation of the virtual library in a computer system.

No additional excess claim fees are submitted since the fees previously submitted are sufficient to cover the additional claims in view of the withdrawn claims.

Claim Rejections - 35 USC § 101

The Examiner has rejected claim 1-3:

"... under 35 USC § 101 because the claimed invention is directed to non-statutory

subject matter. The claims are drawn to non-functional descriptive material. The claims are drawn to data representations of a virtual library of molecules... The libraries are mere presentations of information or abstract ideas which have not been practically applied. (see, e.g. *In re Warmerdam*, 33 F.3 1354, 1361, 31 USPQ 2d 1754, 1760 (Fed. Sir. 1994) (descriptive material *per se* is not patent eligible subject matter.)) No physical molecules are actually created or synthesized, and the data generated by the computer implemented method is merely a list of data structures meeting particular limitations and thresholds. See also the Report on Comparative Study in New Technologies Carried Out Under Trilateral Project..."

Applicants respectfully disagree with the Examiner's analysis of the claims as set out above. In particular, Applicant's submit that the Examiner's characterization of the claims as: non-functional descriptive material, data representations, mere presentations of information, and data structures is incorrect for the reasons set out below. The court in *In re Warmerdam* found that the dispositive issue in that case was "...whether the claim is for a process that goes beyond simply manipulating "abstract ideas" or "natural phenomena." Applicants do not claim either a natural phenomena or a manipulation of abstract ideas. With reference to the present case, an abstract idea may well be that be that there might be some way of characterizing molecular components in such a way that the characteristics of combinations of the molecular components could be assessed. An even more specific, but still abstract, idea might be to utilize some form of metric to characterize the molecular components. These ideas standing by themselves are the type of abstract ideas which may be deemed non-statutory under Warmerdam.

Subsequent to Warmerdam, the Federal Circuit summarized the prohibition against the

patenting of abstract ideas in *ATT & T Corp. V. Excel Communications Inc.*, 172 F.3d 1352, 50 USPQ 2d 1447 (Fed. Cir. 1999). This decision (also written by Judge Plager who wrote Warmerdam) discusses the modicum of usefulness that a claimed invention must have to meet the statutory requirement. In particular, the court noted that information derived from the organization of data by a Boolean operation meets the usefulness requirement:

> "The PIC indicator represents information about the call recipient's PIC, a useful, non-abstract result that facilitates differential billing of long distance calls made by an IXC's subscriber.

Applicants submit that the claims presented more than fully meet the standard set forth both in *Warmerdam* and in *ATT & T*. The virtual library of the present application represents information about molecular structural components, a useful, non-abstract result that facilitates a hitherto impossible type of searching. The present application, provides a tangible, concrete and useful method of achieving the goals of the abstract ideas mentioned above.

In part of the application, Applicants teach a method to validate molecular structural descriptors (metrics) that is; they teach a method of identifying which molecular descriptors usefully characterize molecular structures across a range of structures and activities. Those descriptors which are characterized as valid obey the neighborhood rule and are associated with a characteristic neighborhood distance.

However, a knowledge of the valid descriptors is not sufficient in and of itself, to build a searchable library. Applicants have further taught how to construct the virtual library in such a way that the properties of product molecules (those which can be assembled from the component parts) can be searched without the necessity of actually generating the product structures. The

structure of the virtual library is what makes such searching possible. The virtual library is inventive, it is not abstract, and it is not just a data structure or representation as suggested by the Examiner.

Applicants respectfully submit that it is just such practical applications that are envisaged as rendering a method statutory subject matter under the statute and relevant jurisprudence. The Examiner has also referenced the Trilateral Project in the office action and additionally mentioned the Project and reach through-claims at the interview and in the Interview Summary. Since no rejection is presently of record with respect to reach-through claims, Applicants believe it is premature to make any response.

Applicants respectfully request that the Examiner withdraw the 35 USC § 101 rejections.

Claim Rejections - 35 USC § 102

The Examiner has rejected claims 1-3:

"...under 35 U.S.C. 102(b) as being anticipated by Cramer, III (USP 5,307,287)." The Examiner suggests that Cramer: "...discloses virtual libraries of molecules that could be created wherein the libraries comprise information about the possible structures such as molecular descriptors, characterization data, and common core features."

Applicants are unaware of any disclosure in the '287 patent which deals with virtual libraries. The '287 patent teaches Comparative Molecular Field Analysis (CoMFA) which compares the structures of compounds having different activities in the same biological assay in an attempt to discover how differences in molecular structure affect the activity. The shape of each molecular structure is defined by the steric and electrostatic fields between a probe and each atom in the structure calculated in a three dimensional grid around the structures. The '287 patent

is a continuation of U.S. Patent 5,025,388 and teaches that molecular structures not used to generate solution coefficients from a series of known molecules can be compared to the known molecules using the CoMFA methodology. However, there is no disclosure of virtual libraries as taught and claimed in the present application. Finally, there is no teaching in the '287 patent of molecular structural descriptors validated as possessing a neighborhood property, one of the key elements used in the construction of Applicants' virtual library.

For the foregoing reasons, Applicants respectfully request that the Examiner withdraw the 102(b) rejection.

The Examiner has rejected claims 1-3:

"...under 35 U.S.C. 102(e) as being anticipated by Agrafiotis et al. (5,463,564). The Examiner states that Agrafiotis: "...discloses virtual libraries of molecules that could be created wherein the libraries comprise information about the possible structures such as molecular descriptors, characterization data, and common core features."

Applicants respectfully disagree with the Examiner's analysis. Agrafiotis teaches an iterative method in which each round of chemical analysis is followed up by analysis of the results (using typical prior art analytical methods such as structure activity relationships) and programming of a robotic synthesizer to make new compounds. There is no searching of possible combinatorially derivable product molecules to find molecules having similar properties as is taught by Applicants in the use of their virtual library.

In fact, Agrafiotis' '564 patent specifically does not deal with virtual libraries of combinatorially derivable product molecules. Agrafiotis is concerned with the physical molecules

which he can synthesize. Even in that regard, Agrafiotis teaches away from the use of combinatorial libraries at Col. 5, lines 1-7:

> According to the present invention, a directed diversity chemical library is not the same as a combinatorial chemical library. As discussed above, a combinatorial chemical library comprises a plurality of chemical compounds which are formed by combining, in every possible way for a give compound length (i.e., the number of building blocks in a compound) a set of chemical building blocks.

Col 5, lines 14-

> In contrast, a directed diversity chemical library comprises a plurality of chemical compounds which are formed by selectively combining a particular set of chemical building blocks. Thus, whereas discovery using combinatorial chemical libraries tends to be scattershot and random (essentially constituting a "needle in a haystack" research paradigm), the use by the present invention of directed diversity chemical libraries results in an optimization approach which is focused and directed.

It is exactly the "...scattershot and random approach (essentially constituting a "needle in a haystack" research paradigm)..." that Applicants have overcome by their ability to search the virtual library of this invention for product compounds which will have desired characteristics. On this basis alone, Applicants submit that Agrafiotis can not anticipate Applicants' invention.

However there is another equally important reason that Agrafiotis can not anticipate Applicants' invention. That reason is the fact that Agrafiotis does not utilize or suggest the utilization of validated molecular structural descriptors. Applicants' specification teaches that unless one uses validated descriptors, any selection of molecules is essentially equivalent to a

random selection. Two great advances were disclosed in Applicants' specification and are reflected in the claims, namely: 1) a method for determining whether a descriptor was valid; and 2) a disclosure of validated descriptors possessing a neighborhood property. No method which analyzes molecular structures without disclosing a method to validate and use validated descriptors in that method can anticipate Applicants' method. Accordingly, Agrafiotis et al. can not anticipate Applicants' invention, and Applicants respectfully request the Examiner to withdraw the 102(e) rejection.

Applicants submit that they have adequately addressed all grounds for rejection raised by the Examiner and respectfully request that a timely Notice of Allowance be issued in this case.

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Respectfully submitted,

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